

Qualitative Compound Report

Analysis Info

Analysis Name D:\Data\ggc\NFC-F6 F18-26_P1-F-8_01_7287.d
Method lc_qtof_directospos.m
Sample Name NFC-F6 F18-26
Comment Sv: DCM + MeOH
ML Uhrig

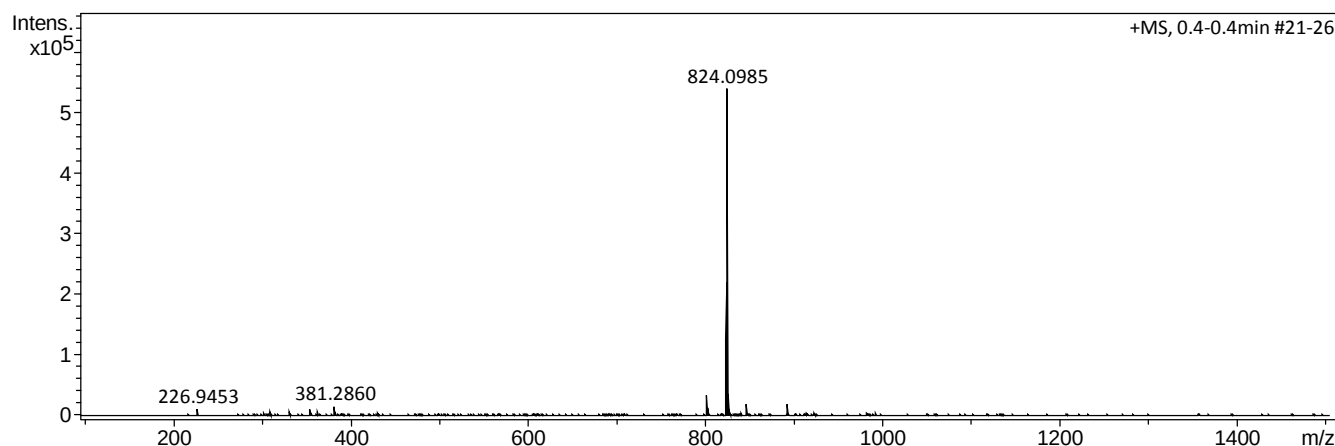
Acquisition Date 5/30/2023 9:33:54 AM

Operator ELB
Instrument micrOTOF-Q II



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
824.0985	1	C24H15N23NaO11	824.1214	27.7	8.0	1	0.00	28.5	even	ok
	2	C24H11N21NaO13	824.0737	-30.1	8.3	2	0.00	29.5	even	ok
	3	C25H15N21NaO12	824.1101	14.1	10.4	3	0.00	28.5	even	ok
	4	C24H10N25O11	824.0986	0.1	10.7	4	100.00	32.5	even	ok
	5	C24H14N19O16	824.0860	-15.2	11.0	5	0.00	27.5	even	ok
	6	C24H7N27NaO8	824.0863	-14.8	11.3	6	0.00	34.5	even	ok
	7	C24H19N17NaO16	824.1088	12.4	11.5	7	0.00	23.5	even	ok
	8	C25H18N19O15	824.1224	29.0	11.5	8	0.00	26.5	even	ok
	9	C25H19N15NaO17	824.0976	-1.2	12.1	9	62.56	23.5	even	ok
	10	C25H14N17O17	824.0748	-28.8	12.3	10	0.00	27.5	even	ok
	11	C26H15N19NaO13	824.0989	0.4	12.9	11	84.93	28.5	even	ok
	12	C26H19N13NaO18	824.0863	-14.8	13.1	12	0.00	23.5	even	ok
	13	C25H10N23O12	824.0874	-13.5	13.3	13	0.00	32.5	even	ok
	14	C26H18N17O16	824.1112	15.4	13.7	14	0.00	26.5	even	ok
	15	C27H23N13NaO17	824.1227	29.3	13.9	15	0.00	22.5	even	ok
	16	C25H7N25NaO9	824.0751	-28.5	14.0	16	0.00	34.5	even	ok
	17	C27H19N11NaO19	824.0751	-28.5	14.6	17	0.00	23.5	even	ok
	18	C24H22N15O19	824.1211	27.4	15.1	18	0.00	21.5	even	ok
	19	C25H22N13O20	824.1099	13.7	15.4	19	0.00	21.5	even	ok
	20	C27H15N17NaO14	824.0877	-13.2	15.5	20	0.00	28.5	even	ok
	21	C26H10N21O13	824.0761	-27.2	15.9	21	0.00	32.5	even	ok
	22	C27H18N15O17	824.1000	1.7	16.0	22	44.33	26.5	even	ok
	23	C28H23N11NaO18	824.1115	15.7	16.1	23	0.00	22.5	even	ok
	24	C26H22N11O21	824.0986	0.1	16.1	24	89.61	21.5	even	ok
	25	C25H11N27NaO7	824.1227	29.3	16.5	25	0.00	33.5	even	ok
	26	C26H27N9NaO21	824.1214	27.7	16.6	26	0.00	17.5	even	ok
	27	C27H27N7NaO22	824.1101	14.1	17.2	27	0.00	17.5	even	ok
	28	C27H22N9O22	824.0874	-13.5	17.2	28	0.00	21.5	even	ok
	29	C24H6N31O6	824.1112	15.3	17.6	29	0.00	37.5	even	ok
	30	C28H15N15NaO15	824.0764	-26.8	18.1	30	0.00	28.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
	31	C28H27N5NaO23	824.0989	0.4	18.1	31	76.12	17.5	even	ok
	32	C29H23N9NaO19	824.1002	2.1	18.4	32	34.95	22.5	even	ok
	33	C28H18N13O18	824.0887	-11.9	18.5	33	0.00	26.5	even	ok
	34	C28H22N7O23	824.0762	-27.2	18.6	34	0.00	21.5	even	ok
	35	C26H11N25NaO8	824.1115	15.7	19.1	35	0.00	33.5	even	ok
	36	C29H27N3NaO24	824.0877	-13.2	19.4	36	0.00	17.5	even	ok
	37	C26H23N7NaO23	824.0738	-30.1	19.5	37	0.00	18.5	even	ok
	38	C25H23N9NaO22	824.0850	-16.4	19.7	38	0.00	18.5	even	ok
	39	C24H3N33NaO3	824.0989	0.4	19.7	39	74.32	39.5	even	ok
	40	C29H26N7O22	824.1125	17.0	19.7	40	0.00	20.5	even	ok
	41	C25H6N29O7	824.1000	1.7	20.1	41	40.99	37.5	even	ok
	42	C24H23N11NaO21	824.0962	-2.8	20.1	42	20.97	18.5	even	ok
	43	C27H14N21O12	824.1125	17.0	20.5	43	0.00	31.5	even	ok
	44	C27H30N5O25	824.1224	29.0	20.5	44	0.00	15.5	even	ok
	45	C30H23N7NaO20	824.0890	-11.6	20.8	45	0.00	22.5	even	ok
	46	C30H27NNaO25	824.0764	-26.8	20.9	46	0.00	17.5	even	ok
	47	C29H18N11O19	824.0775	-25.5	20.9	47	0.00	26.5	even	ok
	48	C28H30N3O26	824.1112	15.4	21.2	48	0.00	15.5	even	ok
	49	C27H11N23NaO9	824.1002	2.1	21.7	49	32.83	33.5	even	ok
	50	C30H26N5O23	824.1013	3.4	21.9	50	13.64	20.5	even	ok
	51	C25H3N31NaO4	824.0876	-13.2	22.1	51	0.00	39.5	even	ok
	52	C31H31NNaO24	824.1128	17.3	22.1	52	0.00	16.5	even	ok
	53	C29H30NO27	824.1000	1.7	22.2	53	38.63	15.5	even	ok
	54	C29H19N15NaO14	824.1128	17.3	22.5	54	0.00	27.5	even	ok
	55	C26H6N27O8	824.0887	-11.9	22.7	55	0.00	37.5	even	ok
	56	C26H26N5O26	824.0861	-15.2	23.2	56	0.00	16.5	even	ok
	57	C28H14N19O13	824.1013	3.3	23.2	57	13.39	31.5	even	ok
	58	C31H23N5NaO21	824.0778	-25.2	23.3	58	0.00	22.5	even	ok
	59	C27H26N3O27	824.0748	-28.8	23.3	59	0.00	16.5	even	ok
	60	C25H26N7O25	824.0973	-1.5	23.3	60	42.22	16.5	even	ok
	61	C24H26N9O24	824.1085	12.1	23.8	61	0.00	16.5	even	ok
	62	C31H26N3O24	824.0901	-10.3	24.2	62	0.00	20.5	even	ok
	63	C28H11N21NaO10	824.0890	-11.6	24.3	63	0.00	33.5	even	ok
	64	C26H3N29NaO5	824.0764	-26.8	24.5	64	0.00	39.5	even	ok
	65	C27H31NNaO27	824.0976	-1.2	24.6	65	48.48	12.5	even	ok
	66	C30H22N11O18	824.1139	18.6	24.7	66	0.00	25.5	even	ok
	67	C26H31N3NaO26	824.1088	12.4	24.8	67	0.00	12.5	even	ok
	68	C30H19N13NaO15	824.1016	3.7	25.1	68	9.83	27.5	even	ok
	69	C27H6N25O9	824.0775	-25.6	25.2	69	0.00	37.5	even	ok
	70	C25H31N5NaO25	824.1200	26.1	25.3	70	0.00	12.5	even	ok
	71	C29H14N17O14	824.0901	-10.3	25.8	71	0.00	31.5	even	ok
	72	C32H26NO25	824.0788	-23.9	26.5	72	0.00	20.5	even	ok
	73	C29H11N19NaO11	824.0778	-25.2	26.9	73	0.00	33.5	even	ok
	74	C32H27N5NaO20	824.1142	19.0	26.9	74	0.00	21.5	even	ok
	75	C31H22N9O19	824.1026	5.0	27.4	75	2.90	25.5	even	ok
	76	C31H19N11NaO16	824.0903	-9.9	27.8	76	0.00	27.5	even	ok
	77	C30H14N15O15	824.0788	-23.9	28.5	77	0.00	31.5	even	ok
	78	C26H34NO29	824.1211	27.4	28.5	78	0.00	10.5	even	ok
	79	C33H27N3NaO21	824.1029	5.3	29.6	79	1.95	21.5	even	ok
	80	C24H27N5NaO26	824.0836	-18.1	29.7	80	0.00	13.5	even	ok
	81	C33H30NO24	824.1152	20.3	29.7	81	0.00	19.5	even	ok
	82	C27H7N29NaO4	824.1128	17.3	30.0	82	0.00	38.5	even	ok
	83	C32H22N7O20	824.0914	-8.6	30.0	83	0.02	25.5	even	ok
	84	C32H19N9NaO17	824.0791	-23.6	30.5	84	0.00	27.5	even	ok
	85	C28H10N25O8	824.1139	18.6	30.6	85	0.00	36.5	even	ok
	86	C30H15N19NaO10	824.1141	18.9	32.1	86	0.00	32.5	even	ok
	87	C34H27NNaO22	824.0917	-8.3	32.2	87	0.04	21.5	even	ok
	88	C28H7N27NaO5	824.1016	3.7	32.4	88	8.33	38.5	even	ok
	89	C25H30NO30	824.0847	-16.8	32.5	89	0.00	11.5	even	ok
	90	C33H22N5O21	824.0802	-22.3	32.7	90	0.00	25.5	even	ok
	91	C29H10N23O9	824.1026	5.0	33.1	91	2.55	36.5	even	ok
	92	C24H30N3O29	824.0959	-3.1	33.4	92	12.23	11.5	even	ok
	93	C31H18N15O14	824.1152	20.2	33.5	93	0.00	30.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
94		C31H15N17NaO11	824.1029	5.3	34.7	94	1.73	32.5	even	ok
95		C29H7N25NaO6	824.0903	-10.0	34.9	95	0.00	38.5	even	ok
96		C33H23N9NaO16	824.1155	20.6	35.3	96	0.00	26.5	even	ok
97		C30H10N21O10	824.0914	-8.7	35.7	97	0.02	36.5	even	ok
98		C24H35NNaO29	824.1187	24.5	35.9	98	0.00	7.5	even	ok
99		C32H18N13O15	824.1040	6.6	36.1	99	0.38	30.5	even	ok
100		C34H26N5O20	824.1166	21.9	37.2	100	0.00	24.5	even	ok
101		C32H15N15NaO12	824.0917	-8.3	37.4	101	0.03	32.5	even	ok
102		C30H7N23NaO7	824.0791	-23.6	37.5	102	0.00	38.5	even	ok
103		C34H23N7NaO17	824.1043	6.9	38.0	103	0.23	26.5	even	ok
104		C31H10N19O11	824.0802	-22.3	38.4	104	0.00	36.5	even	ok
105		C33H18N11O16	824.0927	-7.0	38.8	105	0.21	30.5	even	ok
106		C35H26N3O21	824.1053	8.2	39.9	106	0.04	24.5	even	ok
107		C33H15N13NaO13	824.0804	-22.0	40.0	107	0.00	32.5	even	ok
108		C35H23N5NaO18	824.0930	-6.7	40.7	108	0.30	26.5	even	ok
109		C34H18N9O17	824.0815	-20.7	41.5	109	0.00	30.5	even	ok
110		C36H26NO22	824.0941	-5.4	42.7	110	1.29	24.5	even	ok
111		C31H11N23NaO6	824.1155	20.6	42.9	111	0.00	37.5	even	ok
112		C36H23N3NaO19	824.0818	-20.3	43.4	112	0.00	26.5	even	ok
113		C32H14N19O10	824.1166	21.9	43.7	113	0.00	35.5	even	ok
114		C34H19N13NaO12	824.1168	22.2	45.3	114	0.00	31.5	even	ok
115		C32H11N21NaO7	824.1043	6.9	45.5	115	0.19	37.5	even	ok
116		C33H14N17O11	824.1053	8.2	46.3	116	0.03	35.5	even	ok
117		C35H22N9O16	824.1179	23.5	46.6	117	0.00	29.5	even	ok
118		C35H19N11NaO13	824.1056	8.6	48.0	118	0.02	31.5	even	ok
119		C33H11N19NaO8	824.0930	-6.7	48.0	119	0.24	37.5	even	ok
120		C37H27N3NaO18	824.1182	23.8	48.5	120	0.00	25.5	even	ok
121		C34H14N15O12	824.0941	-5.4	49.0	121	1.06	35.5	even	ok
122		C36H22N7O17	824.1067	9.9	49.3	122	0.00	29.5	even	ok
123		C34H11N17NaO9	824.0818	-20.3	50.6	123	0.00	37.5	even	ok
124		C36H19N9NaO14	824.0944	-5.1	50.7	124	1.43	31.5	even	ok
125		C38H27NNaO19	824.1069	10.2	51.2	125	0.00	25.5	even	ok
126		C35H14N13O13	824.0829	-19.0	51.6	126	0.00	35.5	even	ok
127		C37H22N5O18	824.0954	-3.8	52.1	127	4.46	29.5	even	ok
128		C37H19N7NaO15	824.0831	-18.7	53.3	128	0.00	31.5	even	ok
129		C38H22N3O19	824.0842	-17.4	54.8	129	0.00	29.5	even	ok
130		C35H15N17NaO8	824.1182	23.8	56.1	130	0.00	36.5	even	ok
131		C36H18N13O12	824.1192	25.1	57.0	131	0.00	34.5	even	ok
132		C38H23N7NaO14	824.1195	25.5	58.7	132	0.00	30.5	even	ok
133		C36H15N15NaO9	824.1069	10.2	58.7	133	0.00	36.5	even	ok
134		C37H18N11O13	824.1080	11.5	59.7	134	0.00	34.5	even	ok
135		C39H26N3O18	824.1206	26.8	60.0	135	0.00	28.5	even	ok
136		C37H15N13NaO10	824.0957	-3.4	61.4	136	4.27	36.5	even	ok
137		C39H23N5NaO15	824.1083	11.8	61.4	137	0.00	30.5	even	ok
138		C38H18N9O14	824.0968	-2.1	62.4	138	9.93	34.5	even	ok
139		C40H26NO19	824.1094	13.1	62.7	139	0.00	28.5	even	ok
140		C38H15N11NaO11	824.0845	-17.1	64.0	140	0.00	36.5	even	ok
141		C40H23N3NaO16	824.0971	-1.8	64.1	141	11.35	30.5	even	ok
142		C39H18N7O15	824.0855	-15.8	65.1	142	0.00	34.5	even	ok
143		C41H23NNaO17	824.0858	-15.4	66.8	143	0.00	30.5	even	ok
144		C40H18N5O16	824.0743	-29.4	67.8	144	0.00	34.5	even	ok
145		C37H14N17O8	824.1206	26.7	68.0	145	0.00	39.5	even	ok
146		C39H19N11NaO10	824.1209	27.1	69.5	146	0.00	35.5	even	ok
147		C40H22N7O14	824.1219	28.4	70.5	147	0.00	33.5	even	ok
148		C38H14N15O9	824.1093	13.1	70.6	148	0.00	39.5	even	ok
149		C40H19N9NaO11	824.1096	13.5	72.2	149	0.00	35.5	even	ok
150		C42H27NNaO16	824.1222	28.7	72.2	150	0.00	29.5	even	ok
151		C41H22N5O15	824.1107	14.7	73.2	151	0.00	33.5	even	ok
152		C39H14N13O10	824.0981	-0.5	73.3	152	14.73	39.5	even	ok
153		C41H19N7NaO12	824.0984	-0.2	74.8	153	15.70	35.5	even	ok
154		C40H14N11O11	824.0869	-14.2	75.9	154	0.00	39.5	even	ok
155		C42H22N3O16	824.0995	1.1	75.9	155	10.32	33.5	even	ok
156		C42H19N5NaO13	824.0872	-13.8	77.5	156	0.00	35.5	even	ok

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157		C41H14N9O12	824.0756	-27.8	78.6	157	0.00	39.5	even	ok
158		C43H22NO17	824.0882	-12.5	78.7	158	0.00	33.5	even	ok
159		C43H19N3NaO14	824.0759	-27.4	80.2	159	0.00	35.5	even	ok
160		C41H18N11O10	824.1233	30.0	81.5	160	0.00	38.5	even	ok
161		C42H18N9O11	824.1120	16.4	84.2	161	0.00	38.5	even	ok
162		C44H23N3NaO13	824.1123	16.7	85.8	162	0.00	34.5	even	ok
163		C43H18N7O12	824.1008	2.7	86.9	163	2.65	38.5	even	ok
164		C45H23NNaO14	824.1011	3.1	88.5	164	1.95	34.5	even	ok
165		C44H18N5O13	824.0896	-10.9	89.6	165	0.00	38.5	even	ok
166		C45H18N3O14	824.0783	-24.5	92.3	166	0.00	38.5	even	ok
167		C45H19N7NaO9	824.1136	18.3	97.0	167	0.00	39.5	even	ok
168		C46H22N3O13	824.1147	19.6	97.9	168	0.00	37.5	even	ok
169		C46H19N5NaO10	824.1024	4.7	99.7	169	0.30	39.5	even	ok
170		C47H22NO14	824.1035	6.0	100.7	170	0.07	37.5	even	ok
171		C47H19N3NaO11	824.0912	-8.9	102.4	171	0.00	39.5	even	ok
172		C48H19NNaO12	824.0799	-22.6	105.1	172	0.00	39.5	even	ok
173		C49H23NNaO11	824.1163	21.6	110.8	173	0.00	38.5	even	ok